

Lawrence Livermore National Laboratory

From QCD to Nuclei to Stars



Petr Navratil, Erich Ormand, James Vary, Sofia Quaglioni

Lawrence Livermore National Laboratory, P. O. Box 808, Livermore, CA 94551
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LLNL-PRES-401460

Low-Energy nuclear physics

- Overarching goal:

To arrive at a comprehensive and unified microscopic description of all nuclei and their low-energy reactions from the basic interactions between the constituent protons and neutrons

- This is a lofty and ambitious goal that has been a “Holy Grail” in physics for over fifty years
 - Nuclei are self-bound, two-component quantum many-fermion system
 - Complicated interaction with at least two- and three-nucleon components
 - We seek to describe the properties of “nuclei” ranging from the deuteron to super-heavy nuclei and neutron stars

Our goal is to arrive at an *ab initio* picture for light nuclei and their reactions



Where do we start?

- Quantum chromodynamics (QCD) is the underlying theory for the strong interaction
 - Lattice QCD calculations are far too difficult to do complex nuclei
 - At best they might be able to treat two nucleons
 - They are not capable of providing an accurate nucleon-nucleon interaction in foreseeable future
 - But they can verify that QCD is the correct theory for the strong interaction between hadrons
- We need a theory with point-like nucleons and an interaction based on QCD
 - Effective field theory (EFT) based on the properties of QCD provides an elegant solution with broad predictive power



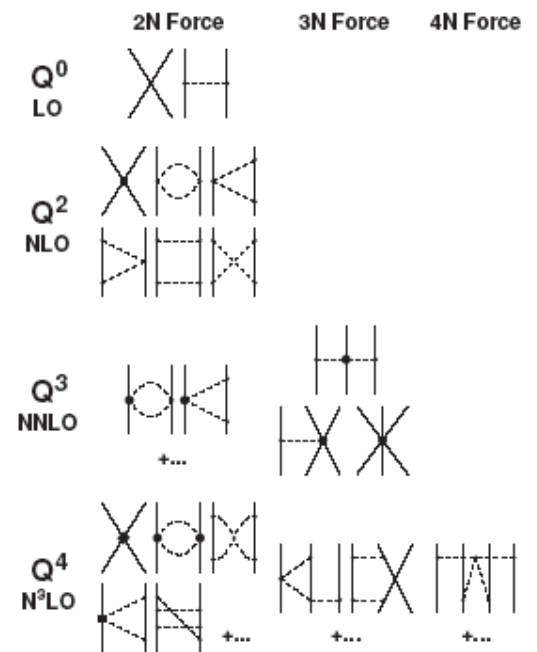
Effective Field Theory

- Based on the symmetries of QCD
 - Degrees of freedom: nucleons + pions
 - Describes pion-pion, pion-nucleon and inter-nucleon interactions at low energies
- Systematic low-momentum expansion to a given order



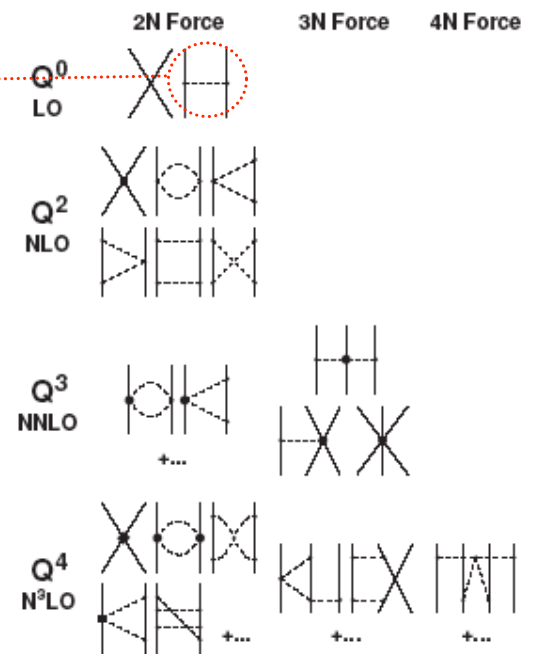
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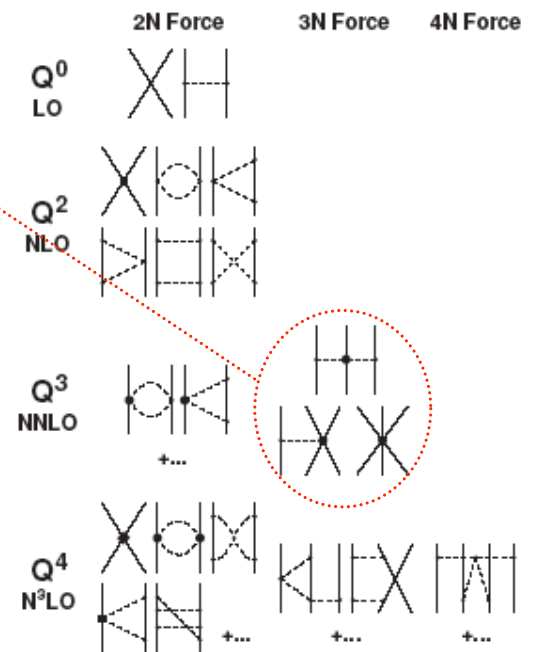
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- Leading order (LO)
 - One-pion exchange



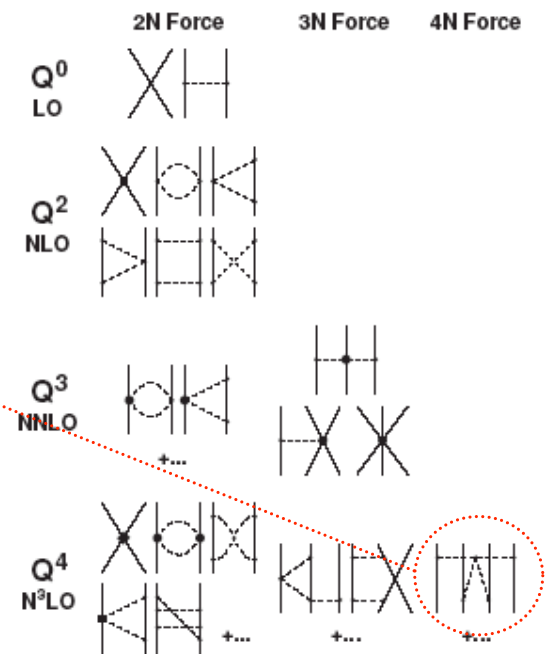
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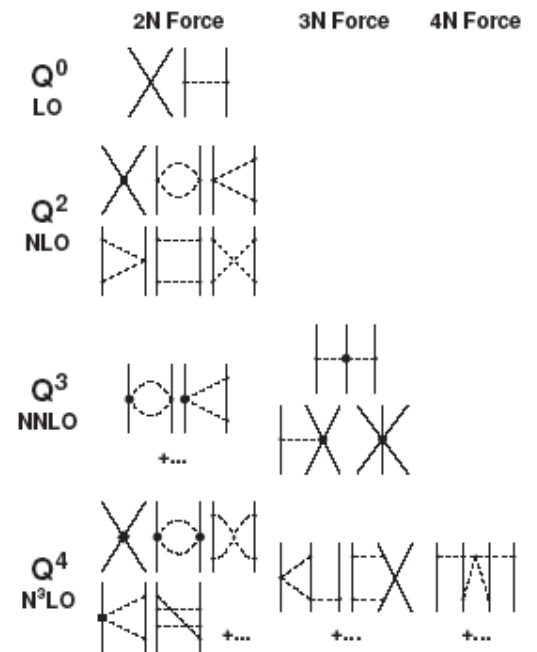
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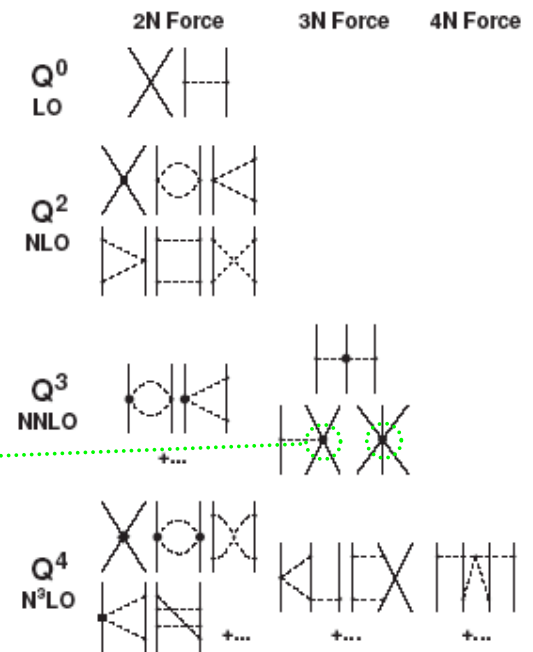
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 - NN parameters enter in the NNN terms etc.



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- Consistency between NN, NNN and NNNN terms
 - NN parameters enter in the NNN terms etc.
- Low-energy constants (LECs)
 - Low-energy theory, integrates out short-range physics
 - Only two NNN and none NNNN low-energy constants up to N^3LO



Why do we need three-nucleon interaction?

- Phenomenological NN potentials provide an accurate fit to NN data



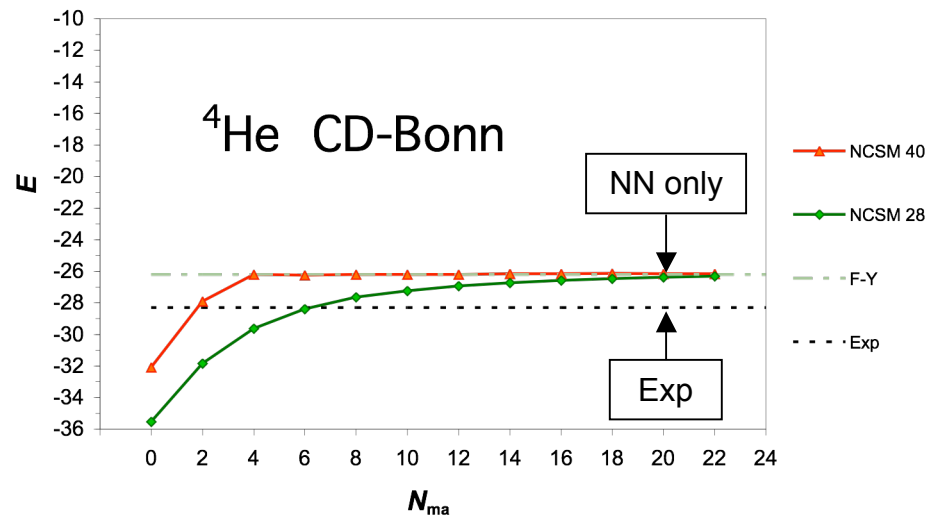
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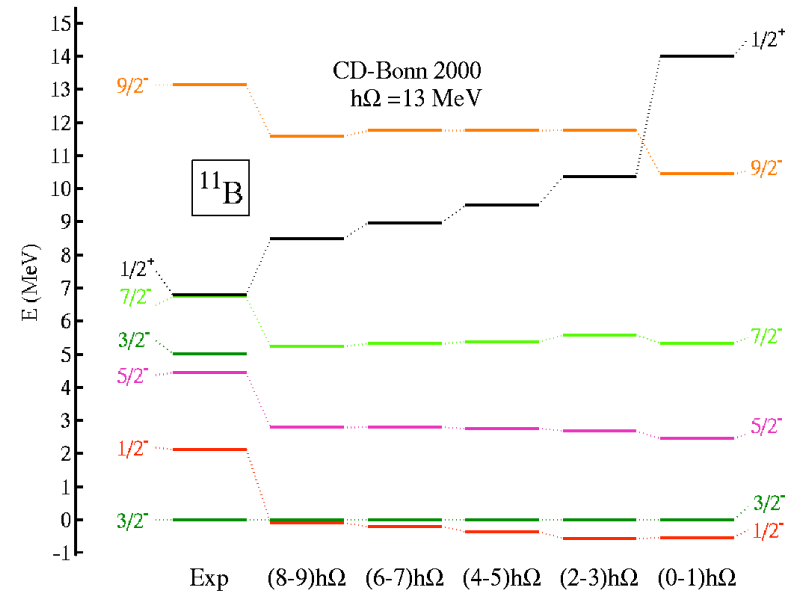
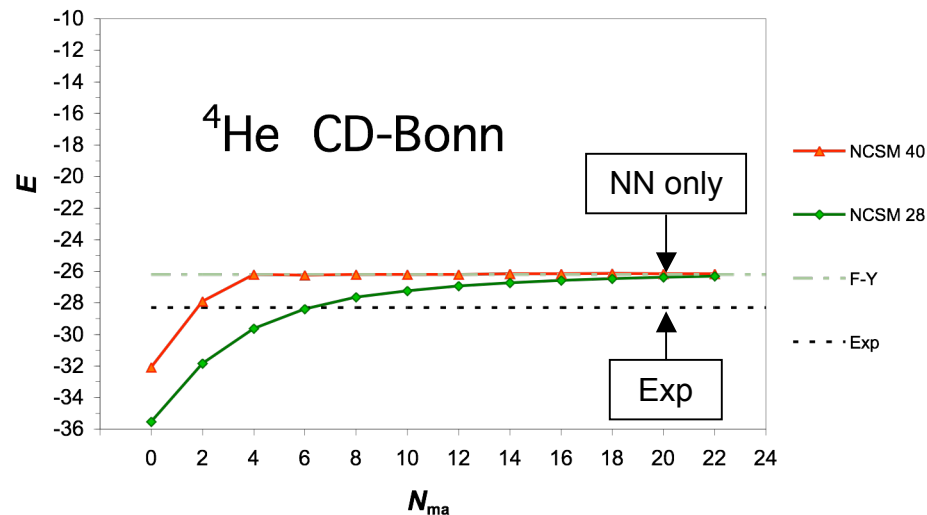
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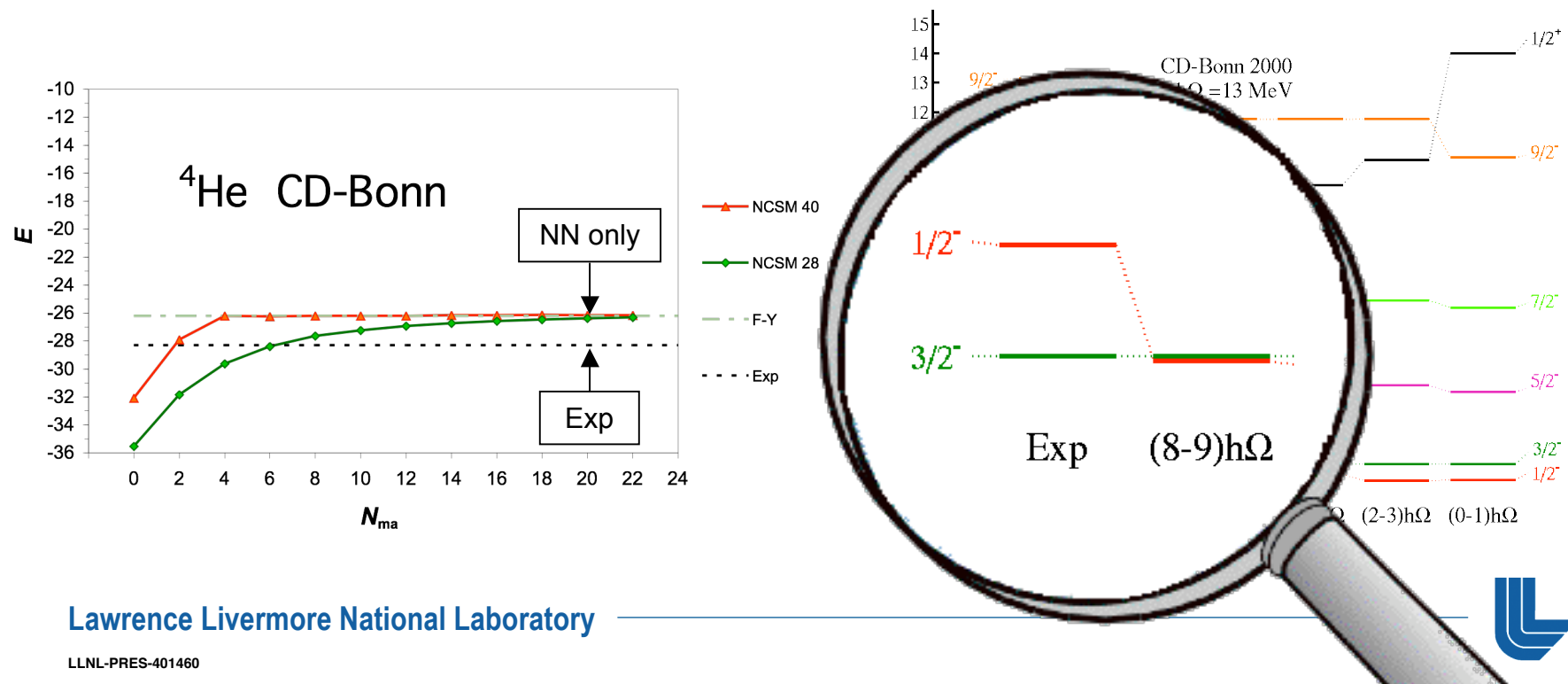
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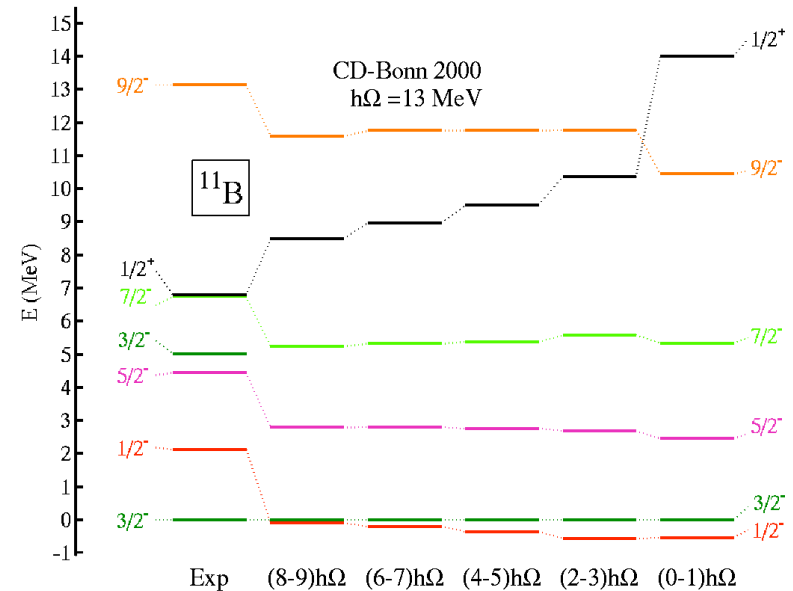
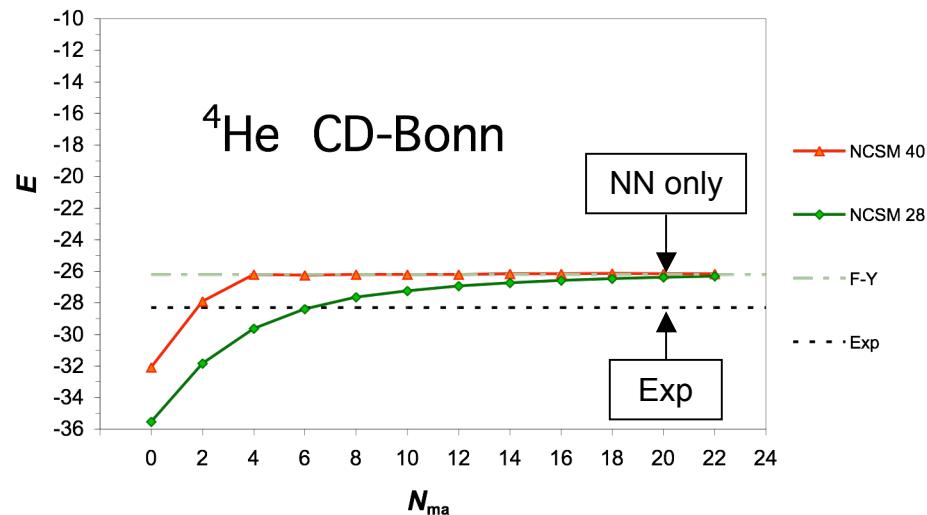
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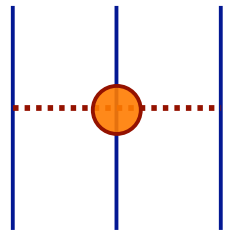
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 - Nuclear structure of p -shell nuclei is wrong
- Predicted by QCD symmetries



The NNN interaction

N²LO

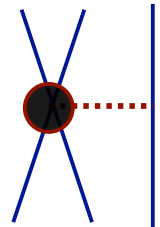


c_1, c_3, c_4

Two-pion exchange

c_1, c_3, c_4 LECs appear in the chiral NN interaction

- Determined in the $A=2$ system

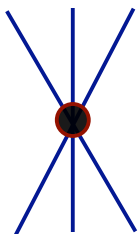


c_D

New!

One-pion-exchange-contact

New c_D LEC



c_E

New!

Contact

New c_E LEC

Must be determined
in $A \geq 3$ system

Nontrivial to include in many-body calculations

– Large-scale computational problem: **ATLAS**

Computational many-body method for nuclei

- *Ab initio* No-Core Shell Model
- Many-body Schrödinger equation
 - A -nucleon wave function
- Realistic nuclear Hamiltonians (NN+NNN)
- Harmonic-oscillator basis
 - Basis size determined by allowed oscillator excitations N_{\max}
 - Construct effective interaction appropriate to the basis
- By construction **convergent to exact solution** with basis enlargement and/or increase in cluster size in the effective interaction

$$H|\Psi\rangle = E|\Psi\rangle$$

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Six-Nucleon Spectroscopy from a Realistic Nonlocal Hamiltonian

P. Navrátil,^{1,2} J. P. Vary,³ W. E. Ormand,¹ and B. R. Barrett⁴

¹Lawrence Livermore National Laboratory, L-414, P.O. Box 808, Livermore, California 94551

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Ab Initio Shell Model Calculations with Three-Body Effective Interactions for p -Shell Nuclei

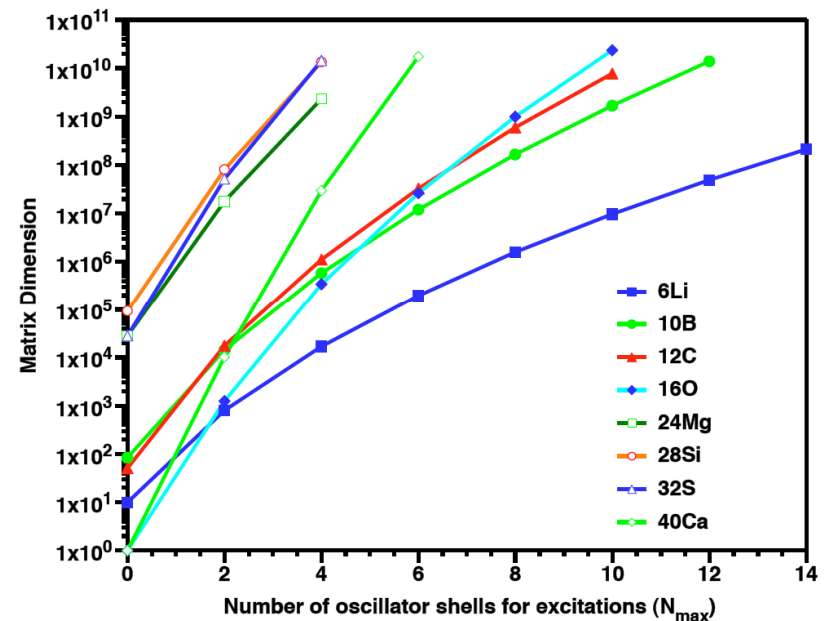
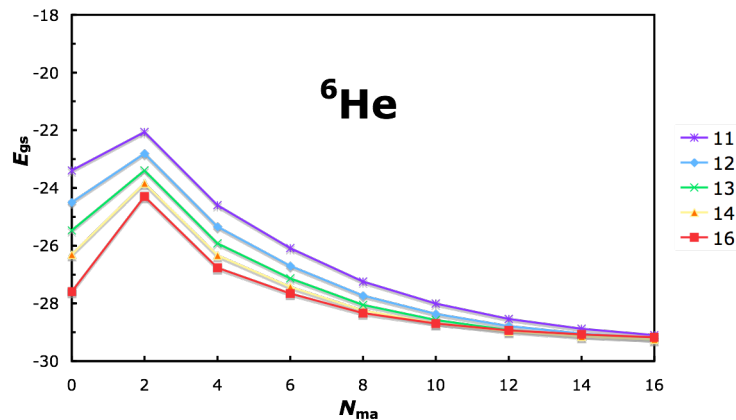
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(Received 19 November 2001; published 2 April 2002)



Computationally demanding problem

- Convergence governed by N_{\max}
- Basis dimension grows with N_{\max}

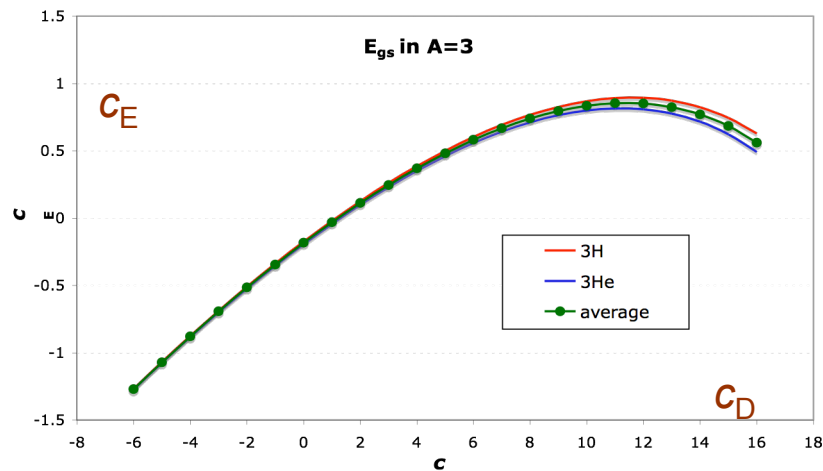


- Typical calculation for ${}^{12}\text{C}$ with $N_{\max}=6$
- Matrix dimension $N_D=32\text{M}$
- Number of NNN matrix elements $\sim 700\text{M}$
- Memory for matrix 8 TB
- $N_{\text{proc}}=3828$
- CPU=11,500 h
- Scales as $N_D^{3/2}$



Determining the three-nucleon interaction: $A=3$ & ${}^4\text{He}$

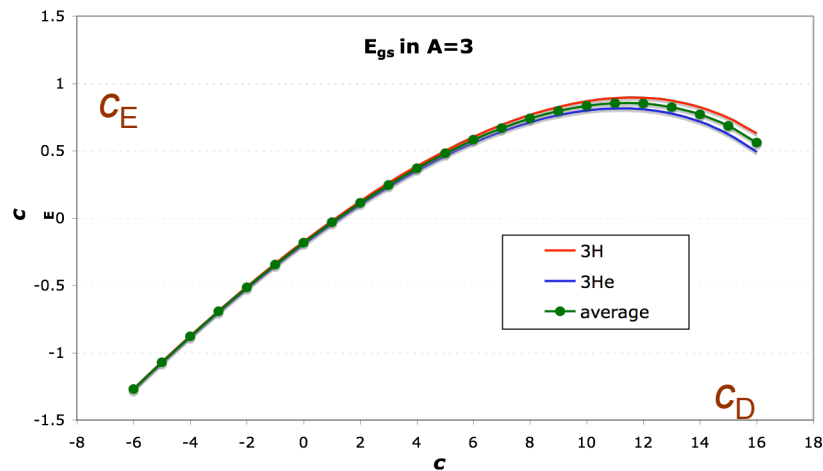
- Constrain c_D , c_E to $A=3$ binding energy



$c_D - c_E$ dependence that fits $A=3$ binding energy

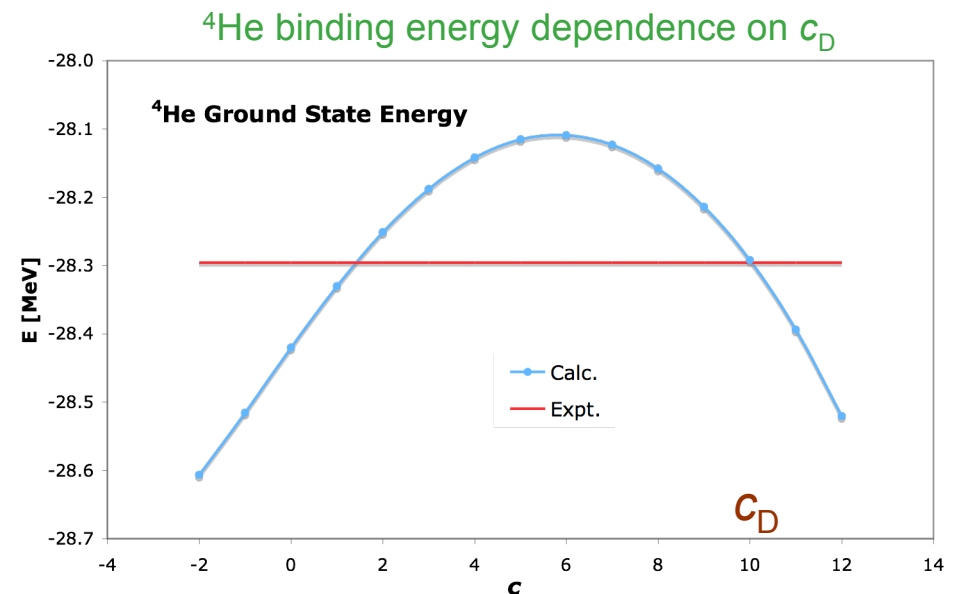
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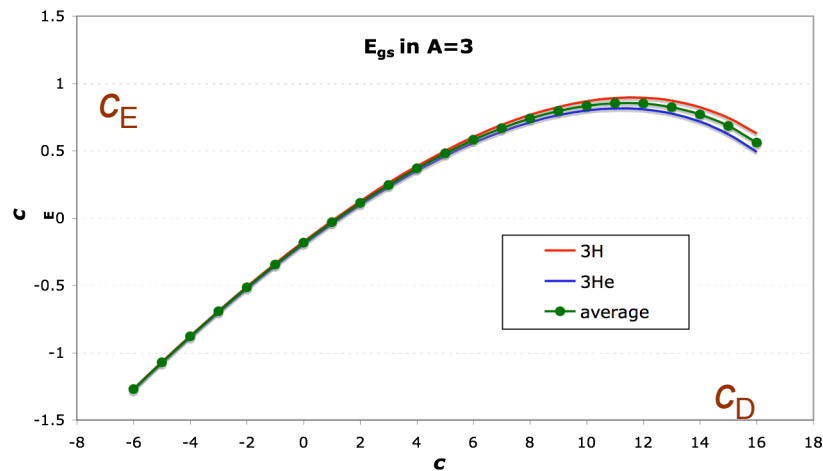
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- Other observables are needed:
 - N-d doublet scattering length
 - Correlated with E_{gs}
- ${}^4\text{He}$ binding energy
- Two combinations of $c_D - c_E$ that fit both $A=3$ and ${}^4\text{He}$ binding energies
 - ${}^4\text{He}$ E_{gs} dependence on c_D weak
 - ${}^4\text{He}$ and $A=3$ binding energies correlated



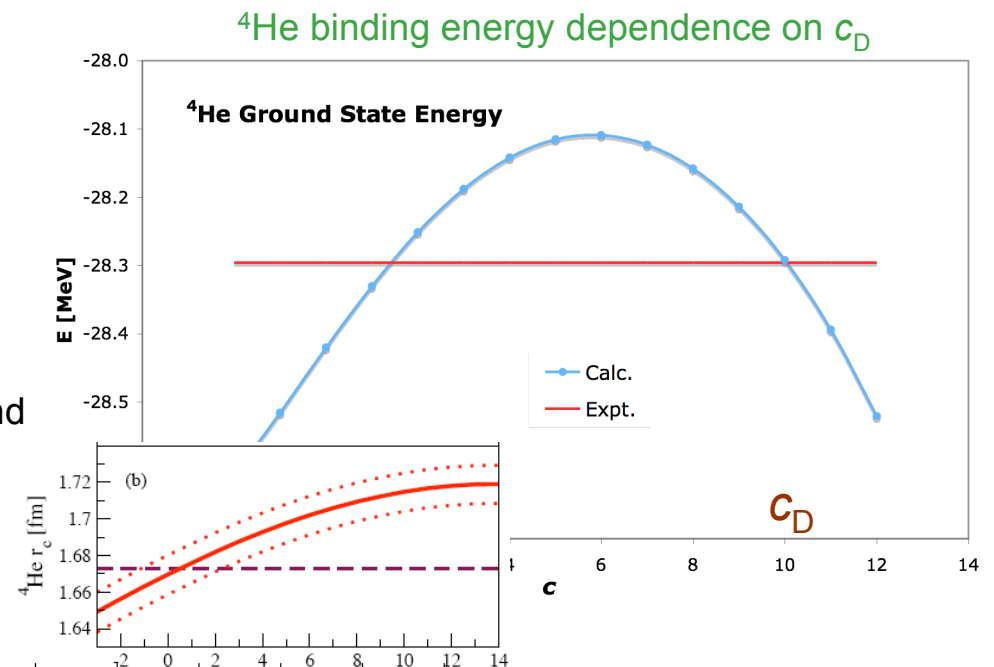
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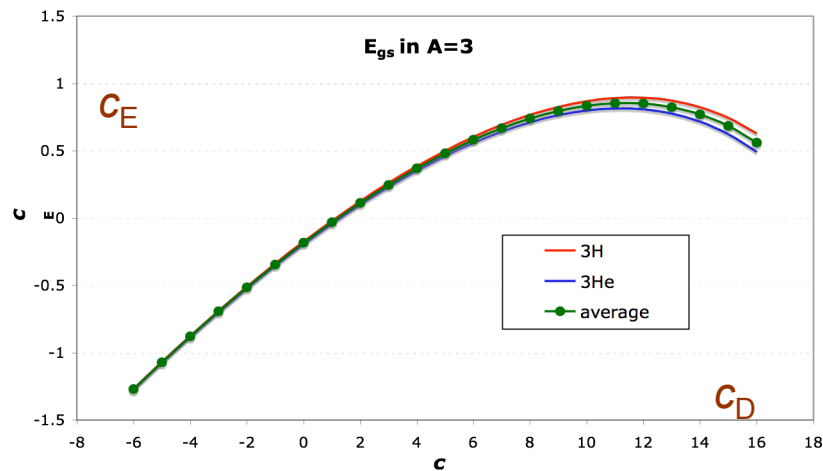
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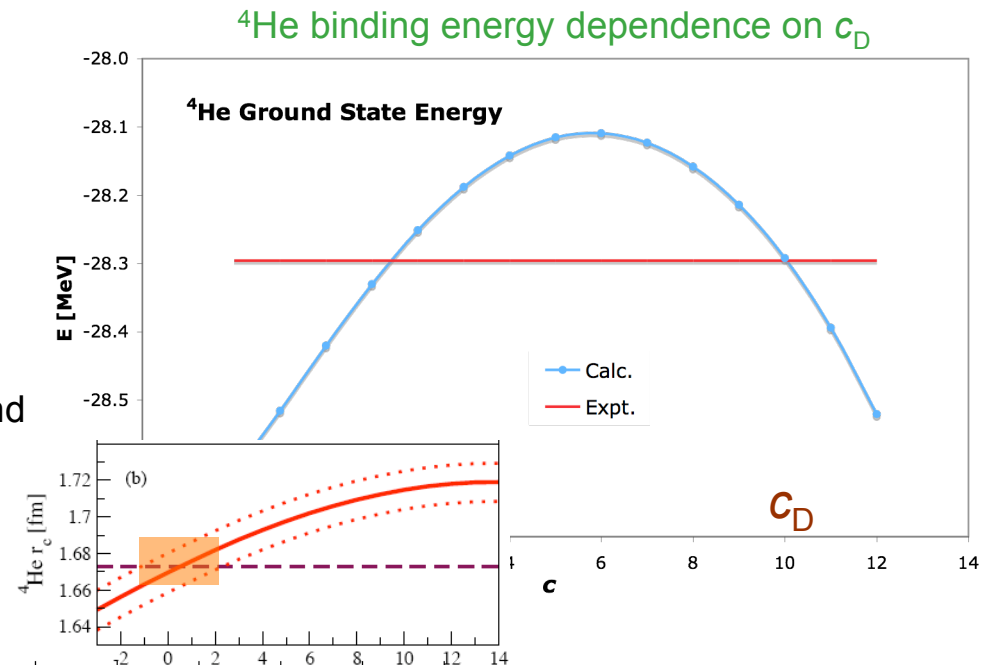
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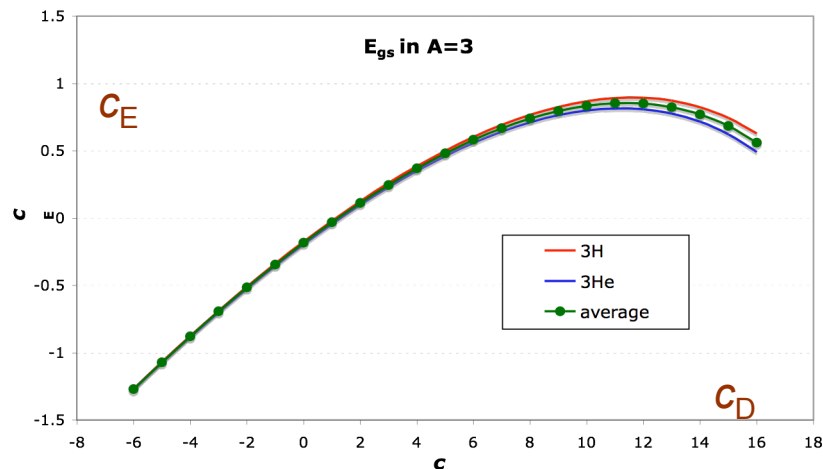
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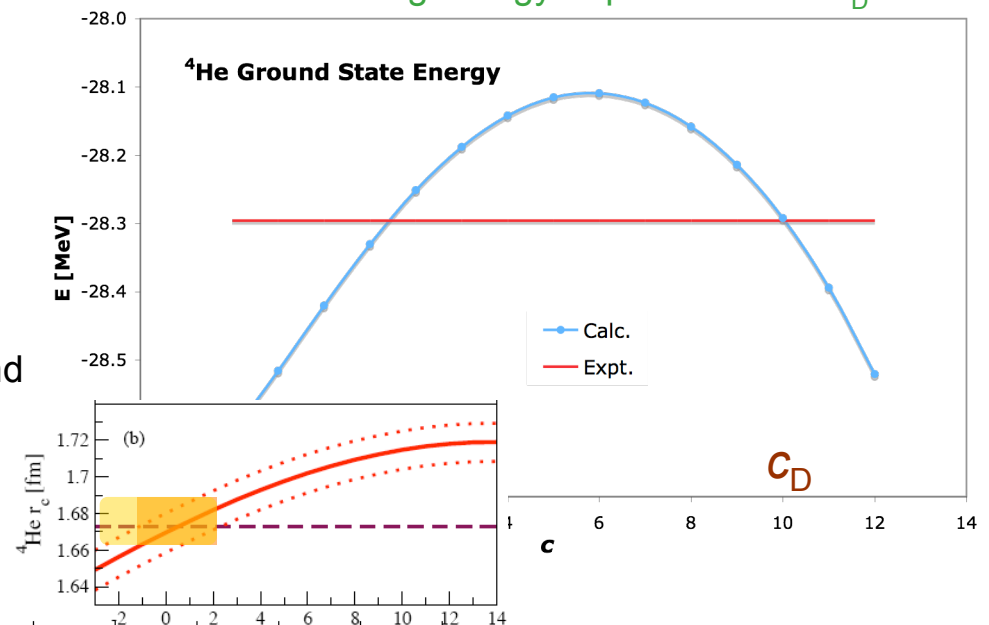


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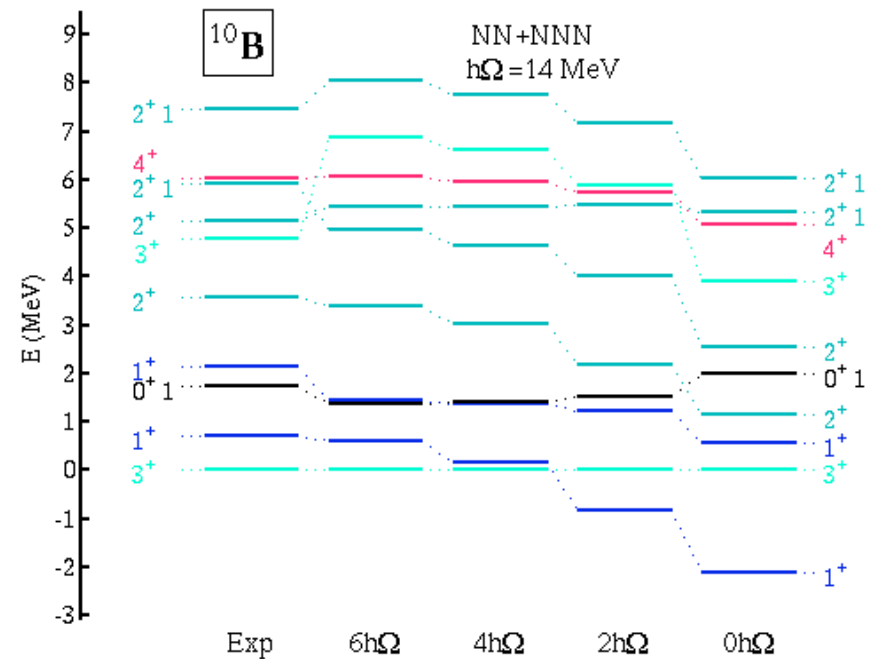
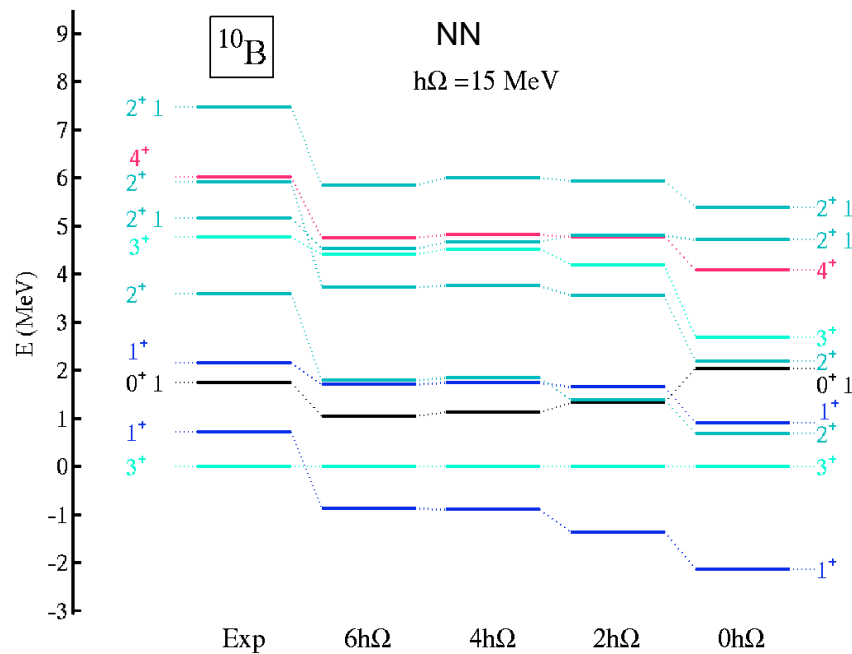
${}^4\text{He}$ binding energy dependence on c_D



What about the structure of p -shell nuclei?

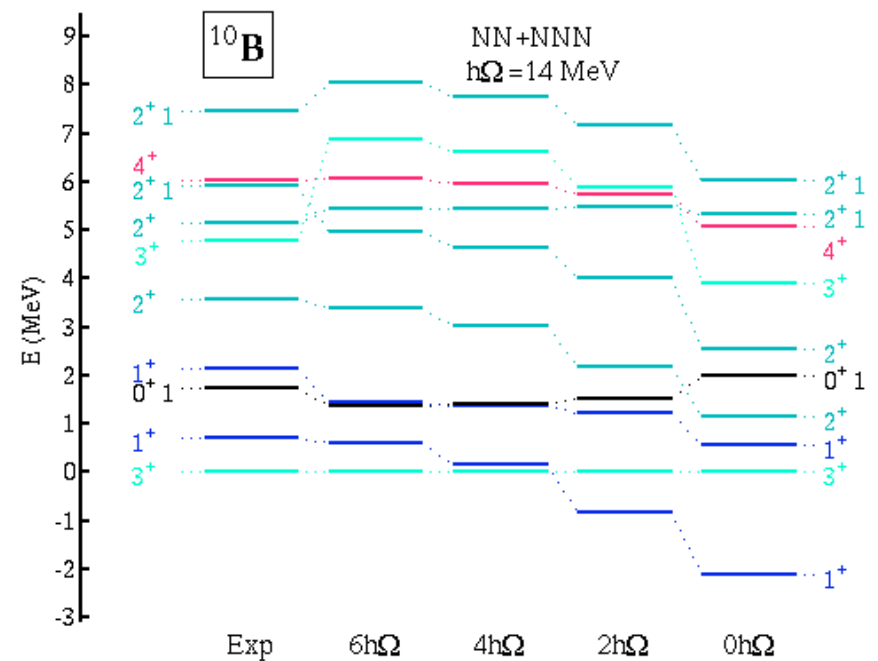
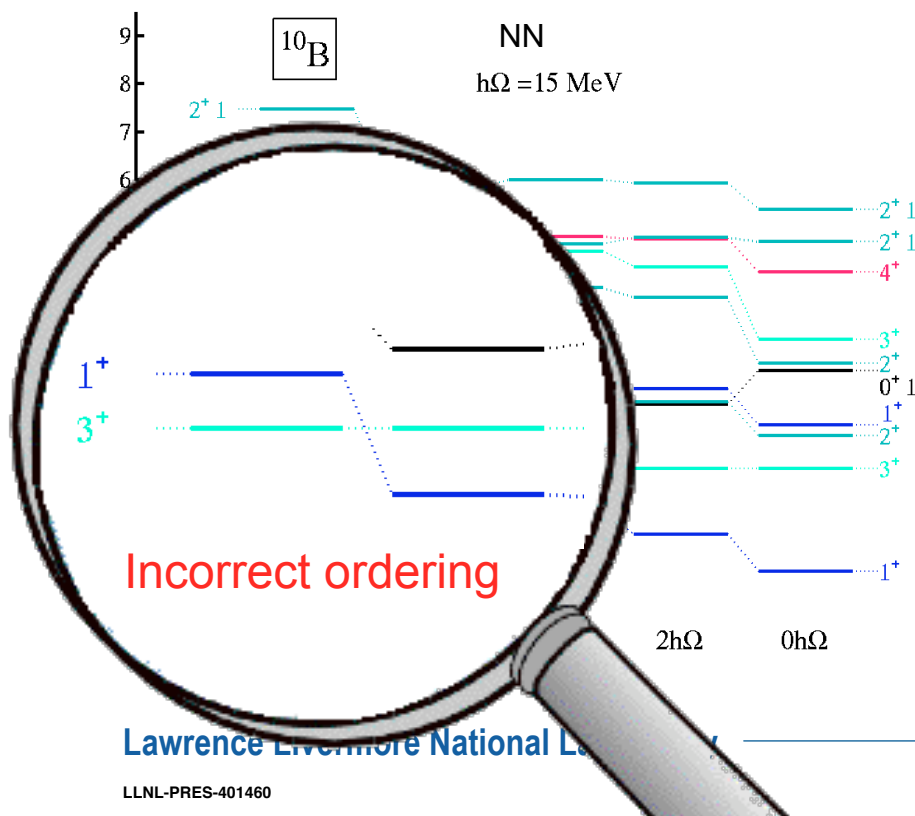
NN is important for heavier *p*-shell nuclei: ^{10}B

- ^{10}B known to be poorly described by standard NN interaction
 - Predicted ground state $1^+ 0$
 - Experiment $3^+ 0$



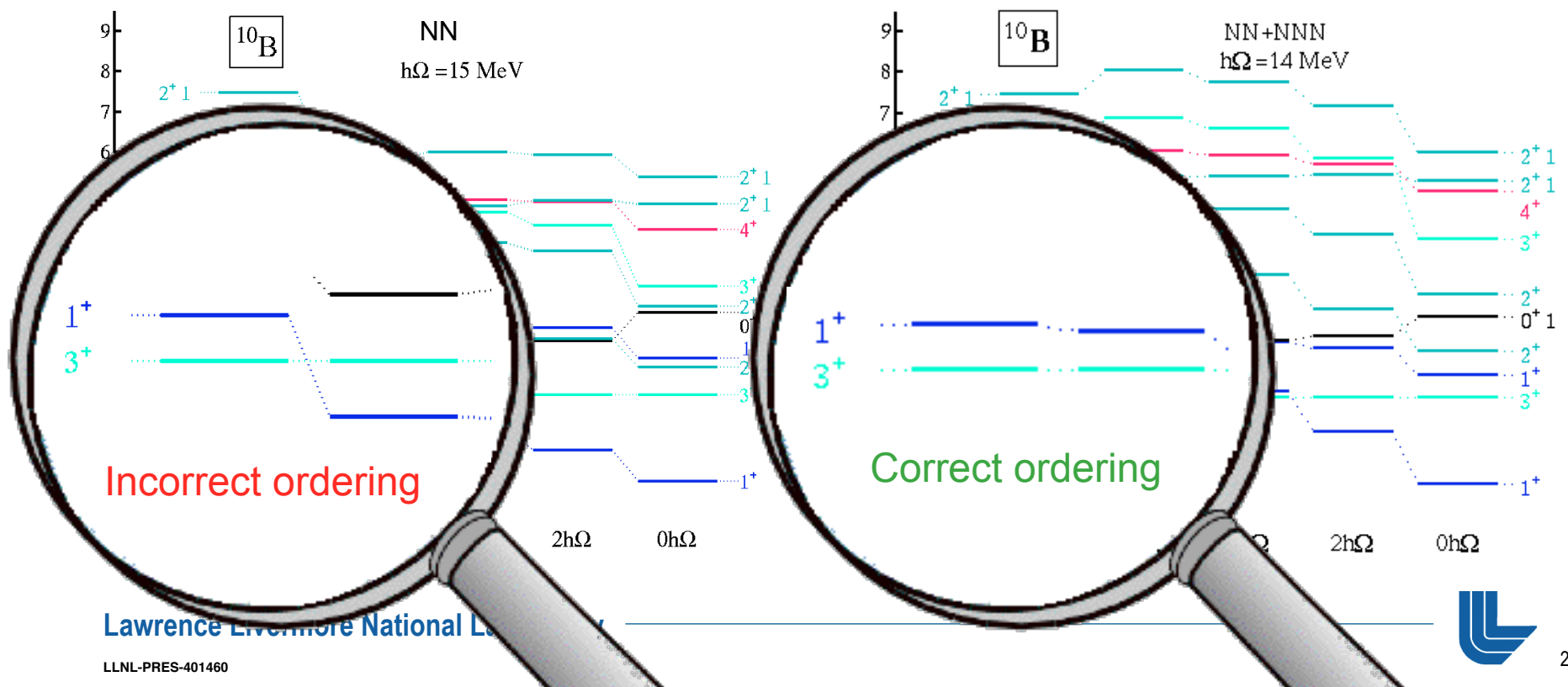
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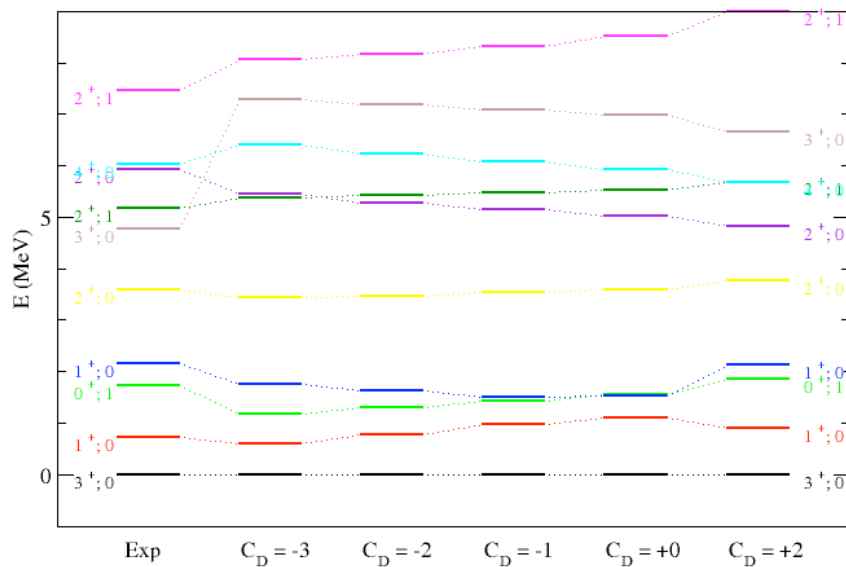
- ^{10}B known to be poorly described by standard NN interaction
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- Chiral NNN fixes this problem



Using the NCSM to determine c_D , c_E : ^{10}B

- ^{10}B properties not correlated with $A=3$ binding energy
- Spectrum shows weak dependence on c_D

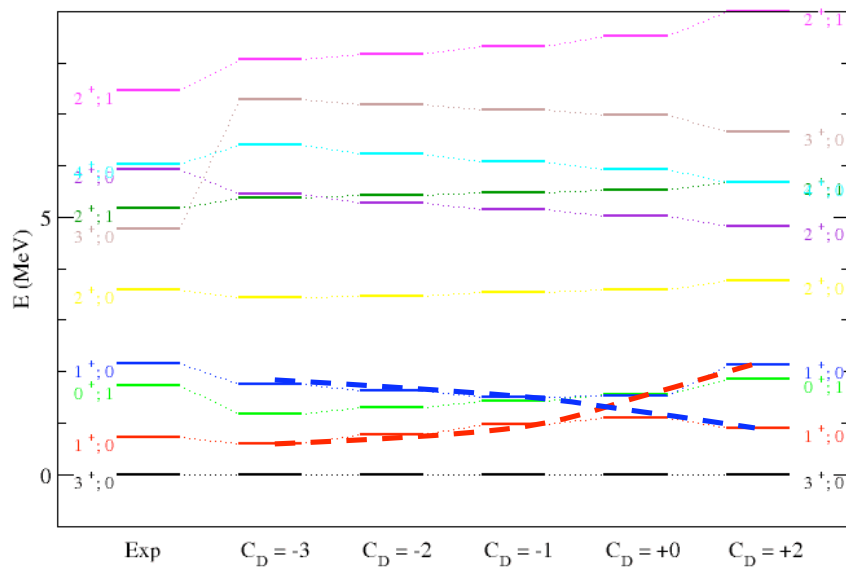
^{10}B NN+NNN c_D dependence for $N_{\text{max}} = 6$, $\hbar\Omega = 15$ MeV



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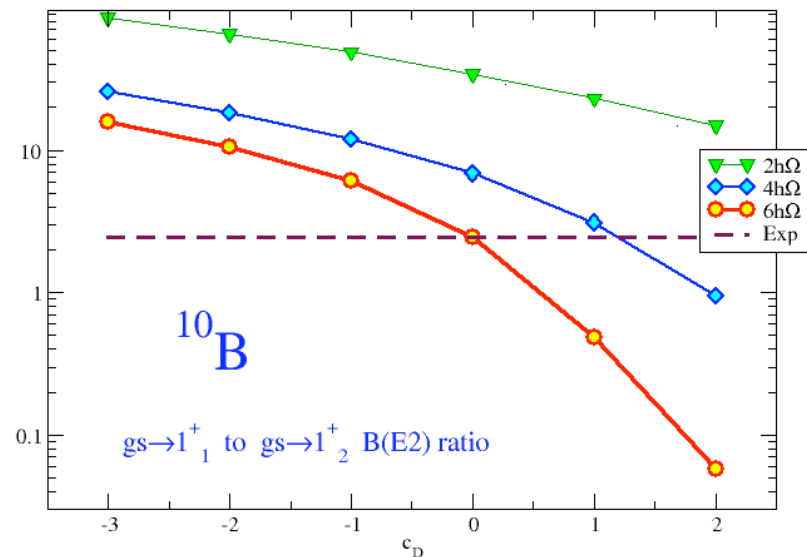
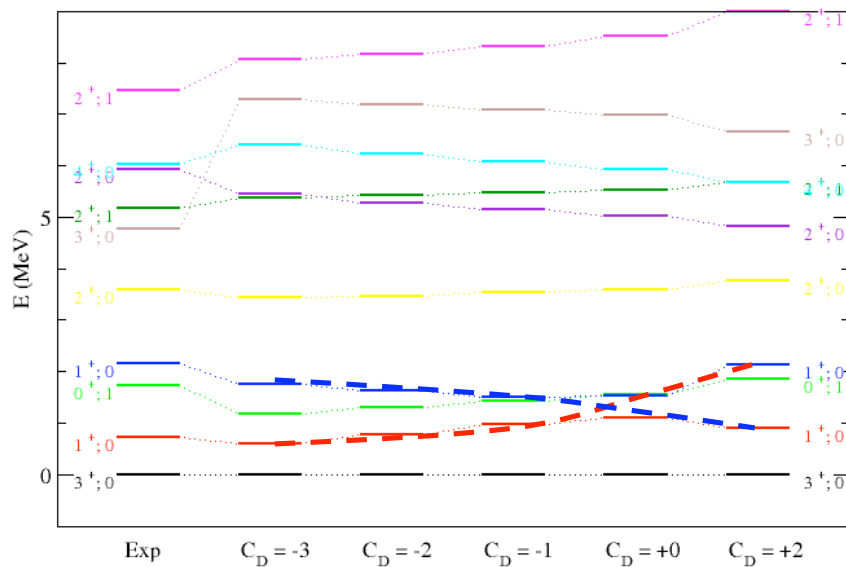
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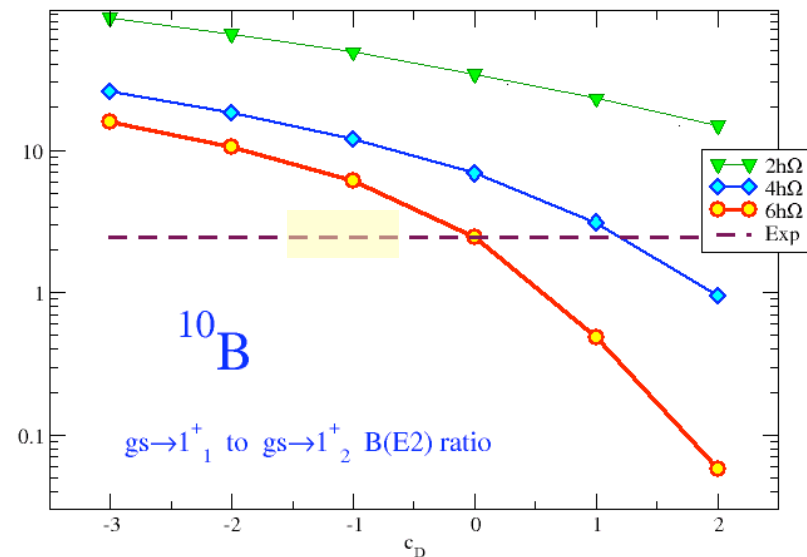
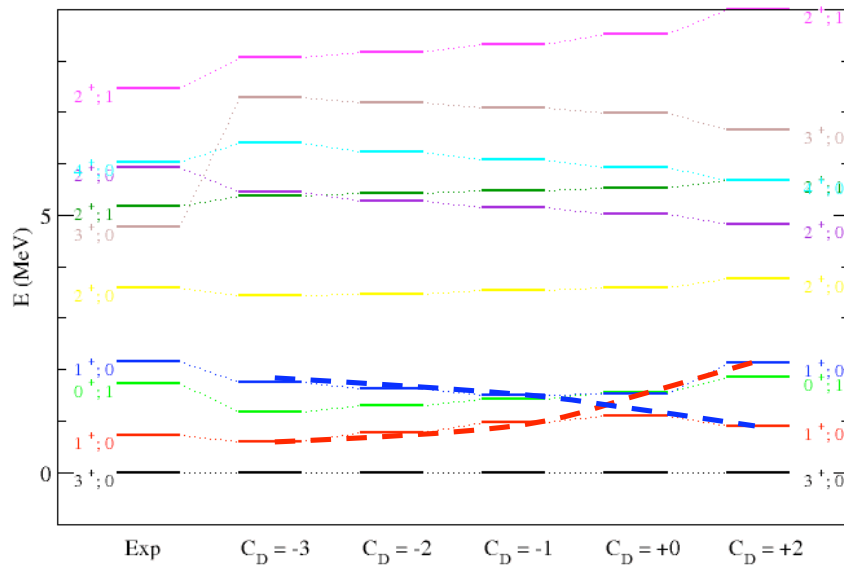


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$c_D \approx -1.5 \sim -0.5$
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^{10}B NN+NNN c_D dependence for $N_{\text{max}} = 6$, $\hbar\Omega = 15$ MeV



Structure of p-shell nuclei with NN+NNN interactions

- NCSM is only method capable to apply the EFT NN+NNN interactions
 - Technically challenging, large-scale computational problem
 - ~4000 processors used in $^{12,13}\text{C}$ calculations
- Applied to constrain the NNN interaction
 - Investigation of $A=3$, ^4He and p -shell nuclei
 - Globally the best results with $c_D \sim -1$
- NNN interaction essential to describe structure of light nuclei

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27 JULY 2007

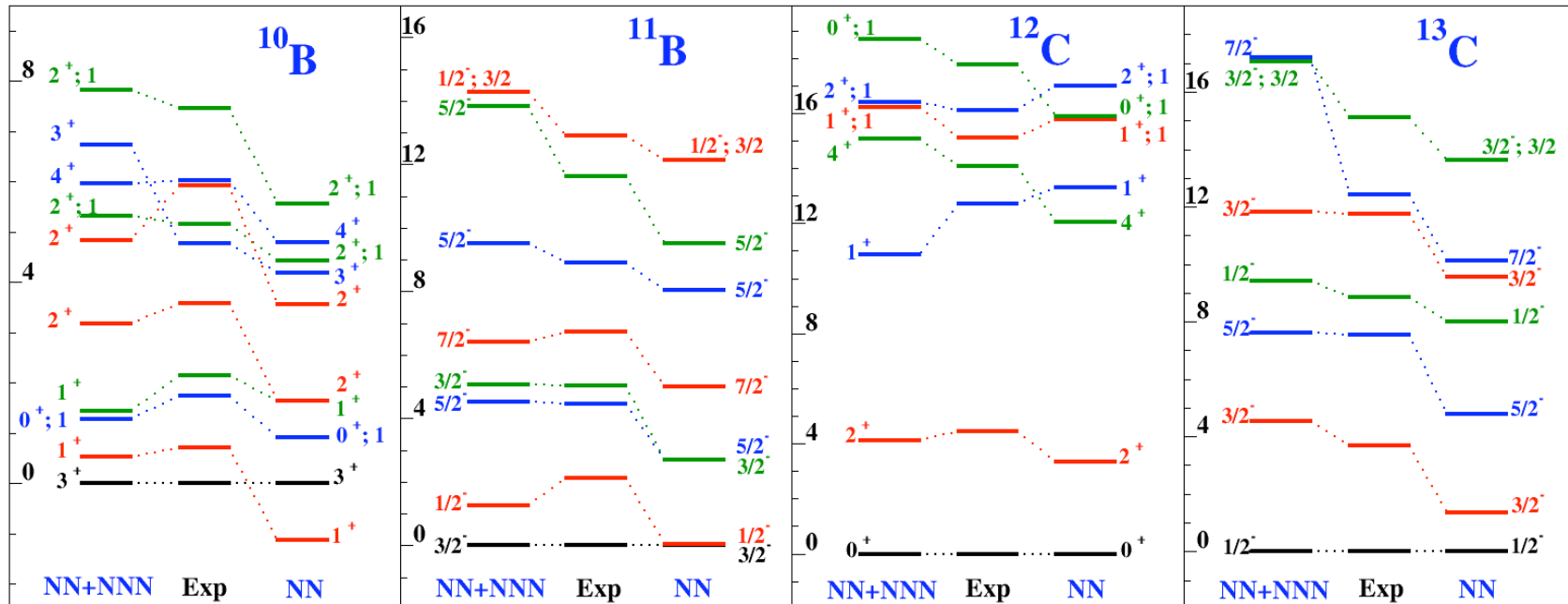
Structure of $A = 10-13$ Nuclei with Two- Plus Three-Nucleon Interactions from Chiral Effective Field Theory

P. Navrátil,¹ V.G. Gueorguiev,^{1,*} J.P. Vary,^{1,2} W.E. Ormand,¹ and A. Nogga³

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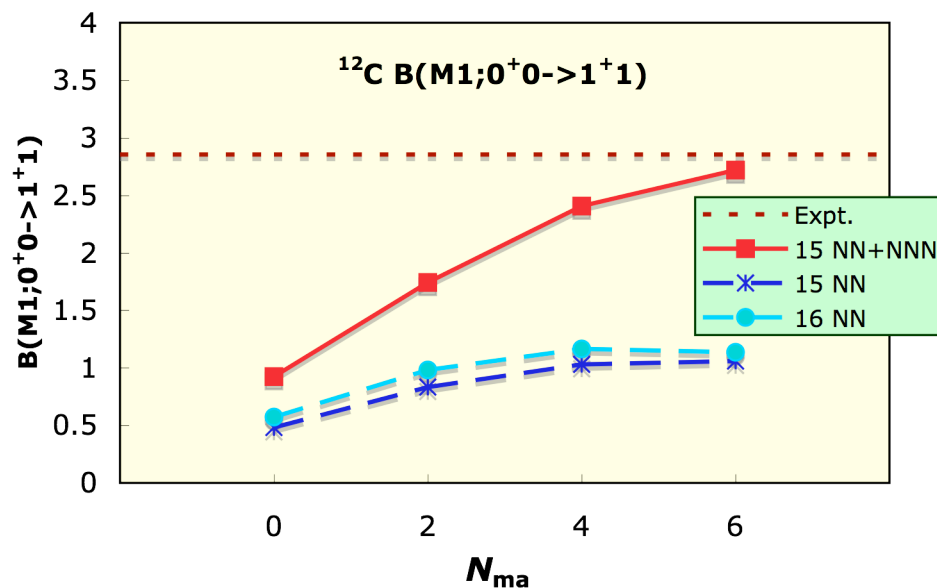
²Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

³Forschungszentrum Jülich, Institut für Kernphysik (Theorie), D-52425 Jülich, Germany
(Received 16 January 2007; published 25 July 2007)



Spin-orbit physics and the NNN interaction

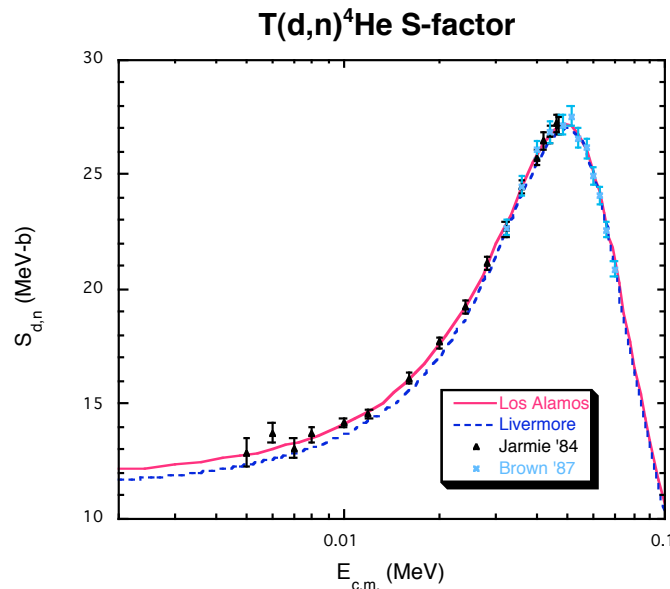
- Gamow-Teller and magnetic dipole transitions are sensitive to NNN
- Sensitivity of $B(M1; 0^+0 \rightarrow 1^+1)$ to the strength of spin-orbit interaction
 - Presence of the NNN interaction
 - Choice of the c_D - c_E LECs



From nuclei to stars:

ab initio approach to light-ion reactions

- *Ab initio* theory of nuclear reactions for $A > 4$ basically non-existent
- Our goal is to provide accurate theoretical cross sections for reactions where measurements are very difficult or impossible
 - Light-ion fusion reactions at low energy:
 - $T(d,n)^4\text{He}$
 - Reactions of importance for astrophysics:
 - $^3\text{He}(\alpha,\gamma)^7\text{Be}$, $^7\text{Be}(p,\gamma)^8\text{B}$, $2\alpha(\alpha,\gamma)^{12}\text{C}$, $^{12}\text{C}(\alpha,\gamma)^{16}\text{O}$

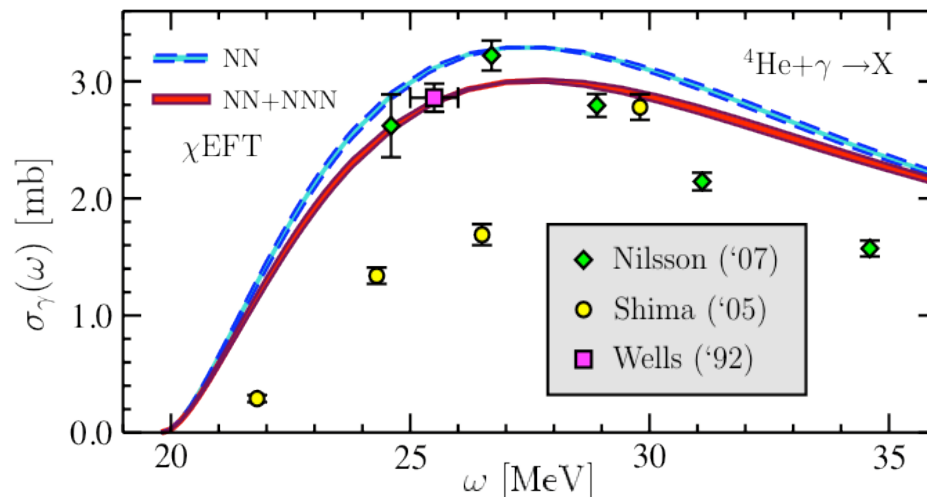


$$\sigma(E) = \frac{S(E)}{E} \exp\left(-\frac{2\pi Z_1 Z_2 e^2}{\hbar \sqrt{2mE}}\right)$$

- low rates due to Coulomb repulsion
- low energies hard to reach in the lab
- large electron screening

Ab initio nuclear reactions: photodisintegration

- Photo-disintegration of ^4He
- Experiment is unclear
 - Can NN+NNN interactions give answers?
- The Lorentz-integral Transform method reduces the continuum problem to a bound-state-like problem

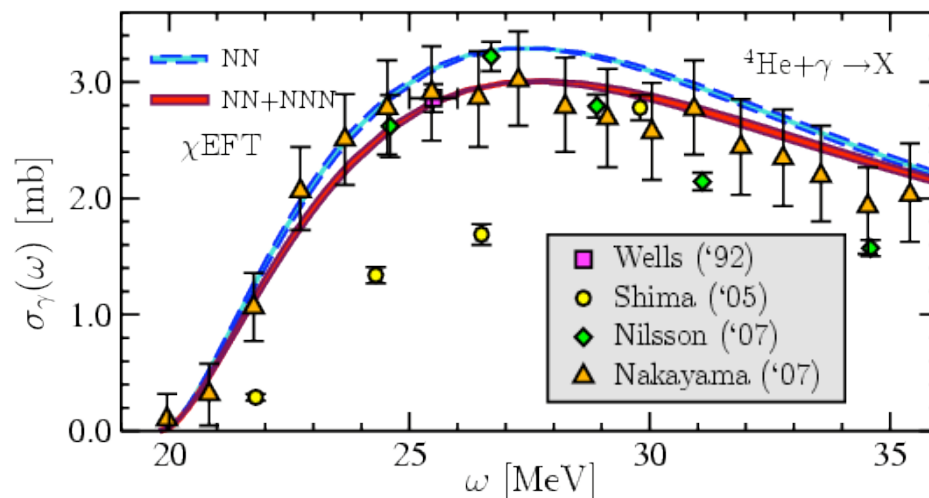


Appreciable effect of the chiral NNN interaction on the cross section
Data by Shima disputed



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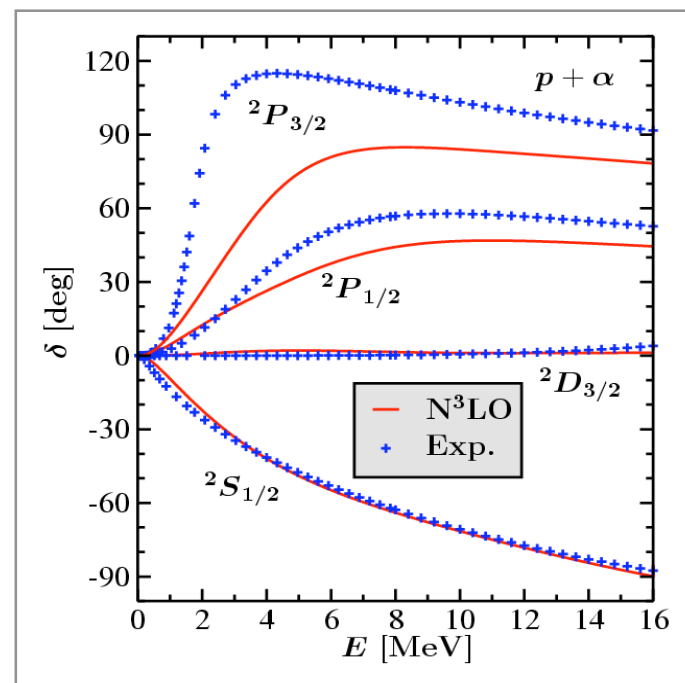
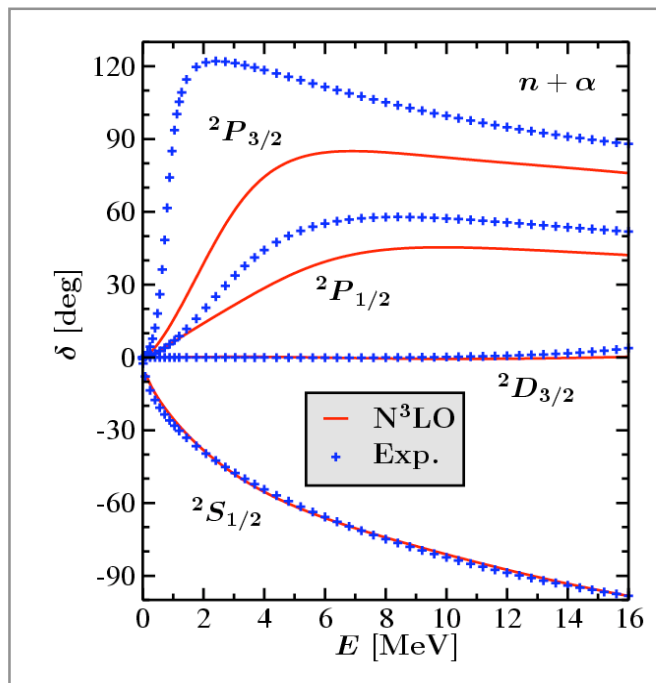


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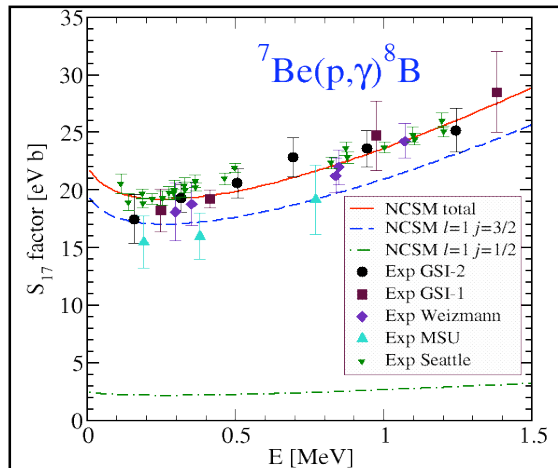


Ab initio reaction theory: nucleons

- We are developing a fully *ab initio* theory for nuclear reactions
 - Based on NCSM & Resonating Group Method (adds continuum)
- $n+{}^4\text{He}$ & $p+{}^4\text{He}$ scattering
 - EFT N^3LO NN potential
 - Agreement with experiment in the ${}^2\text{S}_{1/2}$ channel
 - Disagreement in P-waves due to missing NNN interaction terms

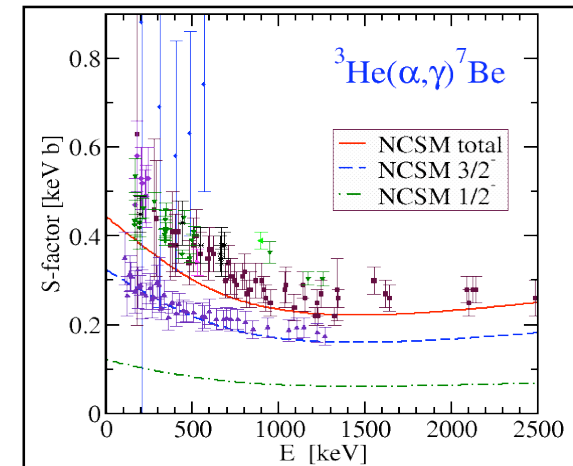


The future



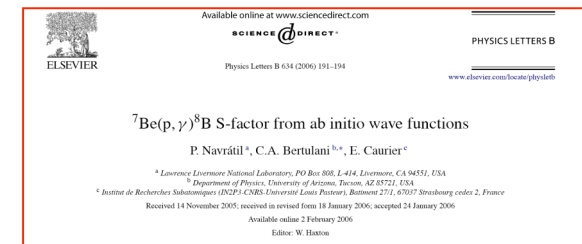
Highlight of DOE
FY08 budget proposal
to congress
for nuclear physics

...
But not fully *ab initio*
...
Can we do better?




The next ATLAS Grand Challenge!

- Augment the *ab initio* NCSM with the RGM technique
 - Includes clustering and resonant plus non-resonant continuum
- From QCD to Nuclei to Stars:
 - Develop a fundamental theory for low-energy nuclear reactions important for astrophysics
- We plan to compute ${}^7\text{Be}(p,\gamma){}^8\text{B}$ and $d(t,n){}^4\text{He}$ this year



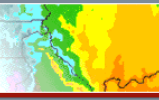
Summary

- High-profile science relevant to DOE/SC/NP mission
 - New insights on the properties of the NNN interaction
 - Responsible for “spin-orbit” physics in nuclei
 - New capability for nuclear reactions
 - Progress towards $^{12}\text{C}(\alpha,\gamma)^{16}\text{O}$
- Four LLNL publications
- Improved capability to compute cross sections for Lab programs
- Outside collaborations
 - J. Vary at ISU
 - Member of the UNEDF SciDAC-2 project



SciDAC
Scientific Discovery through Advanced Computing

assessing
global
climate
change



Office of Science

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Life Sciences
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SciDAC Institutes

Enabling Technologies

Applied Mathematics
Computer Science
Visualization & Data Mgt.

SciDAC Outreach

Participating Orgs

Grant Solicitations

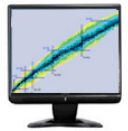
FY2007
FY2006
FY2005
FY2004
FY2001

Collateral Materials

SciDAC Review magazine
'06 Progress Report (pdf)
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A Closer Look at Nuclei
Building a Universal Nuclear Energy Density Functional

Supporting the Low-Energy Nuclear Physics National HPC Initiative

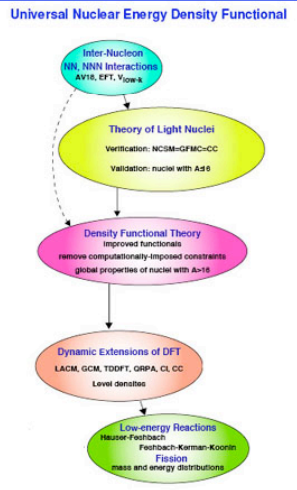
[George F. Bertsch \(project webpage\)](#)
[University of Washington](#)

There are approximately 3,000 known nuclei, most of them produced in the laboratory. It is estimated that additionally up to approximately 6,000 nuclei could in principle still be created and studied in the foreseeable future. An understanding of the properties of these elements is crucial for a complete nuclear theory, for element formation, for properties of stars, and for present and future energy and defense applications. We plan a comprehensive study of all these nuclei, based on the most accurate knowledge of the strong nuclear interaction, the most reliable theoretical approaches, and a massive use of the computer power available at this moment in time, with the view of scaling to the petaflop computers to become available in the near future. Until recently such an undertaking was hard to imagine, and even at the present time such an ambitious endeavor would be far beyond what a single researcher or a traditional research group could carry out. This project will involve theoretical physicists, computer scientists, and students from universities and national laboratories. Our long-term vision is to arrive at a comprehensive and unified description of nuclei and their reactions, grounded in the fundamental interactions between the constituent nucleons. We seek to replace current phenomenological models of nuclear structure and reactions with a well-founded microscopic theory that delivers maximum predictive power with well-quantified uncertainties.

The Energy Density Functional (EDF) is at the heart of the project. EDF theory has been spectacularly successful in condensed matter physics and chemistry, as was recognized in the Nobel Prize awarded to Walter Kohn in 1998. In fact, it was the combined work of many dedicated researchers that culminated in finding a remarkably accurate functional for use in chemistry. Recognizing that the nucleus is composed of fermions, neutrons and protons, EDF is the only tractable theory that can be applied across the entire table of nuclides. The mission of this project is three-fold:

- First, to find an optimal functional using all our knowledge of the nucleonic Hamiltonian and basic nuclear properties.

Universal Nuclear Energy Density Functional



```

graph TD
    A[Inter-Nucleon  
NN, NNN Interactions  
AV18, EFT,  $V_{low-k}$ ] --> B[Theory of Light Nuclei  
Verification: NCISIM-GFMC-CC  
Validation: nuclei with  $A \leq 6$ ]
    B --> C[Density Functional Theory  
Improved functionals  
remove computationally-imposed constraints  
global properties of nuclei with  $A \leq 16$ ]
    C --> D[Dynamic Extensions of DFT  
LACM, GCM, TDFT, QRPA, CI, CC  
Level densities]
    D --> E[Low-energy Reactions  
Heuser-Feshbach  
Feshbach-Kerman-Koonin  
Fusion  
mass and energy distributions]
  
```